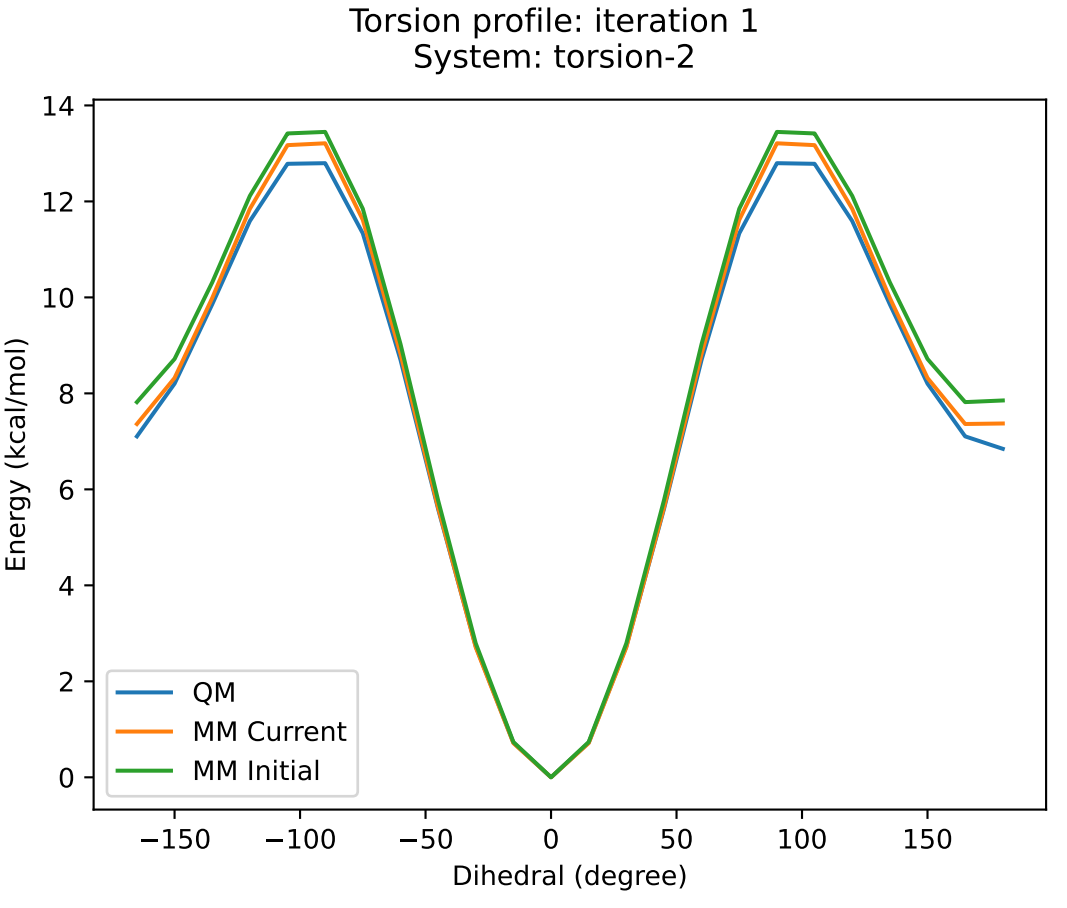
Torsion profile: iteration 1
System: torsion-2
Energy (kcal/mol)
Dihedral (degree)
QM
MM Current
MM Initial
14
12
10
8
6
4
2
0
−150
−100
−50
0
50
100
150